

AIKATERINI VRIZA

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SUMMARY

I am currently a Postdoctoral Appointee at Argonne National Laboratory of the U.S Department of Energy, working towards advancing the way chemistry is performed today by applying cutting edge digital solutions. I was awarded my PhD from the Materials Innovation Factory at the University of Liverpool in 2022 and a Master in Green Chemistry and Sustainable Industrial Technology from the University of York in 2018. Prior to that I was working as an Aviation Engineer for the Hellenic Airforce. I have obtained two Bachelor degrees, one in Electronics Engineering from the Hellenic Airforce Academy and one in Chemistry from the University of Patras. I am a multidisciplinary scientist working in the interface of laboratory automation, chemistry, and computer science. My research vision is to fuse technological advancements to chemistry and materials science to enable for a transition towards a more sustainable and greener society.

EDUCATION

- PhD, Machine learning in Chemistry, Materials Innovation Factory, University of Liverpool & Cambridge Structural Datacenter, Cambridge, 2022
- MSc, Green Chemistry and Sustainable Industrial Technology, University of York, Green Chemistry Center of Excellence , 2018
- BS, Chemistry, University of Patras, 2016 (top 5%)
- BEng, Electronics and Telecommunication Engineering in Aviation Science, 2012 (honors)

WORKING EXPERIENCE

Argonne National Laboratory, USA

Postdoctoral Appointee

September 2022 to current

- Building a self-driving laboratory targeted to the synthesis of polymer electronics (<https://www.anl.gov/cnm/polybot>)
- Incorporate Machine learning components to the autonomous system
- Controlling the robot-equipment and robot-human interactions

Atinary Technologies Inc, Lausanne/Remote

part-time Data Scientist

July 2021 to February 2022

- Developing an AI/ML platform to digitize RD operations and enable self-driving labs that accelerate materials discovery
- Research regarding optimization techniques targeted for experimental chemistry, e.g. incorporating chemical knowledge to the optimizer, effectively searching a constrained chemical space
- Collaborating with IBM Zurich for enabling the acceleration of organic reactions
- Grand applications for start-up funding

JB Morrell Library, York, UK

Customer service-IT

Sept 2017 to August 2018

- Providing IT advice regarding the University resources to the students of the University of York
- Weekend job during my MSc studies

Hellenic Air force, 117 Andravida Military Airbase, Greece

First Lieutenant

July 2011 to Sept 2017

- Served in the Hellenic Military Airforce as an Inspector Electronics Engineer in charge of the electronic department within the 338 squadron, being in charge and leading a technical team of 15 people working on the electronic system of the aircraft F-4E
- Data analysis and anomaly detection for the aircraft avionics system
- Maintained and updated the databases regarding the regular aircraft maintenance procedures
- Aircraft accident investigator. Detected an important materials fault in the aircraft's engine
- Knowledge and application of quality standards and control processes in the domain of aircraft system maintenance

TEACHING AND MENTORING EXPERIENCE

- 2018 to present - Mentoring aviation engineers to pursue a research career abroad
- 2017 to 2021 - Graduate Teaching Assistant at the University of Liverpool for the modules Introduction to Spectroscopy(CHEM170), Physical Chemistry Workshop (CHEM152), Molecular Modelling (CHEM280).
- 2013-2017 Supporting and mentoring young women military aviation engineers for their career development

AWARDS

- Competitive state scholarship from the highest research organization in Greece, the Academy of Athens, for Postgraduate studies in Chemistry, covering all my expenses for studying abroad
- Post graduate research studentship from the Leverhulme Research Center for Functional Materials Design and Cambridge Crystallographic Datacenter
- York University Scholarship to undertake the Master in Green Chemistry and Sustainable Industrial Technology

CONFERENCE PRESENTATIONS

- 4th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry 2021, remote, invited speaker
- 15th International Conference on Materials Chemistry (MC15), remote, poster presentation
- AMLD 2020, Lausanne, AI & Molecular World, speaker
- European UGM and Science Day, The CCDC, Cambridge, Jun 2019, invited speaker

PUBLICATIONS

- **A. Vriza**, H. Chan, J. Xu, Self-Driving Laboratory for polymer electronics: Challenges and Opportunities (under review).
- **A. Vriza**, I. Sovago, D. Widdowson, P. A. Wood, V. Kurlin, N., M. S. Dyer, Molecular Set Transformer: Attending to the co-crystals of the Cambridge Structural Datacenter, Digital Discovery 2022. <https://doi.org/10.1039/D2DD00068G>.
- **A. Vriza**, A. B. Canaj, R. Vismara, L. J. K. Cook, T. D. Manning, M. W. Gaultois, P. A. Wood, V. Kurlin, N. Berry, M. S. Dyer, M. J. Rosseinsky, One class classification as a practical approach for accelerating $\pi - \pi$ co-crystal discovery, Chem. Sci, 2021, 00, 1–3.
- L. Longanesi, F.P. Bouxin, J. Fan, H. Auta, R. Gammons, V.L. Budarin, **A. Vriza**, J. H. Clark & C. J. Chuck, Biomass Conversion and Biorefinery, 2020, <https://doi.org/10.1007/s13399-020-00757-3>.
- **A. Vriza**, A. Kargioti, P.J. Papakanellos, G. Fikioris, Physical Communication, 2018, 31, 133-140.

OTHER SKILLS

Organize Organizing and coordinating seminars for AI in materials science in the Materials Innovation Factory, Program planning in international military exercises

Languages English: professional proficiency. German: conversational. Greek: native

Activities Yoga, Dancing Swing, Hiking in the mountains, Rafting, Paddling

REFERENCES

Dr Jie Xu xuj@anl.gov, Postdoctoral advisor, Research Scientist at Argonne National Laboratory

Dr Matthew Dyer msd30@liverpool.ac.uk, PhD supervisor, Senior Lecturer of Chemistry at the University of Liverpool

Prof Matthew Rosseinsky rossein@liverpool.ac.uk, Project supervisor, Professor and co-founder of the Materials Innovation Factory

Dr Vitaliy Kurlin vitaliy.kurlin@liverpool.ac.uk, Secondary PhD supervisor, Senior Lecturer of Computer Science at the University of Liverpool